

Random loose packing and an order parameter for the parking lot model

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Abstract

We have obtained the random loose packing fraction of the parking lot model (PLM) by taking the limit of infinite compactivity in the two-variable statistical description of Tarjus and Viot for the PLM. The PLM is a stochastic model of adsorption and desorption of particles on a substrate that have been used as a model for compaction of granular materials. An order parameter ρ is introduced to characterize how far from a steady state situation the model is. Thus, configurations with $\rho < 1$ age. We propose that ρ can be a starting point in order to establish a connection between Edwards' statistical mechanics and granular hydrodynamics.

1 Introduction

More than twenty years ago Edwards and Oakeshott proposed a statistical mechanics framework for granular materials in mechanical equilibrium [1]. The idea was to replace the energy by the total volume of the sample V . Thus the entropy of the system is defined as $S = \log \Omega$, where Ω is the number of stable states for a given volume V (and given number of grains N). The quantity equivalent to temperature within this description is the compactivity $\chi = (\partial S / \partial V)^{-1}$. In connection with Edwards proposal, Aste *et al* has found for static packings of spheres an invariant distribution of Voronoi volumes at the grain level [2]. Also, the random close packing fraction ϕ_{rcp} and the random loose packing fraction ϕ_{rlp} have been associated with configurations with $\chi \rightarrow 0$ and $\chi \rightarrow \infty$, respectively [3, 4, 5].

It has been shown recently that two granular samples with the same packing fraction may not have the same properties, and an additional macroscopic variable must be introduced in the statistical description. In reference [6] was found that we can produce two samples with the same ϕ but different stresses. Indeed, the stress tensor σ has been included in a more general statistical description [7] (see [6] and references therein).

We deal in this article with the so called *parking lot model* (PLM) introduced by Nowak *et al* in the context of experiments of compaction of grains [8]. Starting with the statistical mechanics for the PLM proposed by Tarjus and Viot [9], we obtain the random loose packing fraction for this model and introduce an order parameter ρ that characterizes how far from a steady state situation the model is. We propose that a quantity analog to ρ can be used as the order parameter in the continuum description of slow and dense granular flows by Aranson and Tsimring, mediating how solid and fluid is the form of the stress tensor [10, 11].

The PLM is a model of random adsorption and desorption of particles on a substrate. Particles are disorbed with rate p_- and adsorbed with rate p_+ , with a no overlapping condition. For a given initial condition of the substrate, the model converges to a stationary state packing fraction ϕ_e around which it fluctuates. ϕ_e depends only on the ratio $K = p_+/p_-$, which allow us to map the parameter K to Γ or Q of references [8, 12]. For large K we have $\phi_e = 1 - 1/\log K$ [13] and the convergence to a stationary state is very slow, reminiscent of glassy behavior [14]. The PLM is though to represent an average column of grains.

Tarjus and Viot characterized the configurations produced by the PLM with two variables [9]. One of them is the packing fraction ϕ and the other is the insertion probability Φ , which is the available line fraction for a new insertion. Tarjus and Viot recognized the need for an additional variable because of some memory effects observed in experiments that can be reproduced within the PLM if we change K in the course of a Monte Carlo simulation: we can generate two configurations with the same ϕ but with different subsequent evolution and by allowing a variation in K , for a given finite time, we can obtain more dense substrates [15]. Thus, the history of the configuration is encoded in Φ , which is a structure variable [16]. The additional variable Φ is only needed to characterize configurations which are not produced in steady state, since in steady state the insertion probability Φ_e is given by (eq. 2 in [15]):

$$\Phi_e = (1 - \phi) \exp[-\phi/(1 - \phi)]. \quad (1)$$

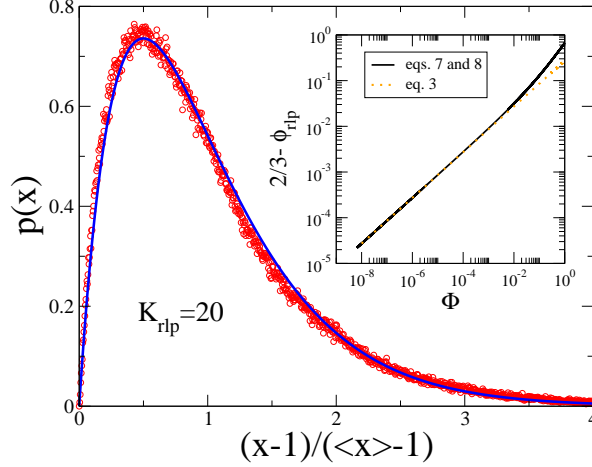


Figure 1: Distribution of Voronoi lengths of the PLM for $K_{rlp} \approx 20$ obtained with Monte Carlo Simulations (circles). The continuum line is a gamma distribution with shape parameter $k = 2$ [2, 20]. In the inset we show $2/3 - \phi_{rlp}$ vs. the insertion probability Φ for the PLM as given by eqs. 7 and 8. The dotted line is equation 3. At $\Phi \approx 0.01$ the difference in ϕ_{rlp} is less than 1% .

2 Results

If A is the total lenght available for a new insertion ($A = \Phi L$, where L is the size of the system), for given N , L and A we have a configurational integral in terms of the gaps h_i (eq. 25 in [9]):

$$Z = \int_0^L \dots \int_0^L dh_i^N \delta \left(L - N - \sum_{i=1}^N h_i \right) \delta \left(A - \sum_{i=1}^N \theta(h_i - 1)(h_i - 1) \right) \quad (2)$$

with θ being the step function. Equation 2 can be solved with a saddle point method in the limit of large N , L and A , with $\phi = N/L$ and $\Phi = A/L$ fixed.

In steady state, for $K = 100$ we have $\Phi \approx 0.01$ [15]. In the limit of small Φ we obtain a random loose packing fraction by taking the limit $\chi \rightarrow \infty$ in the above description (see Appendix):

$$\left(\frac{2}{3} - \phi_{rlp} \right) \approx \sqrt{\frac{2}{27}} \Phi^{1/2}. \quad (3)$$

Since the random loose packing of granular media depends on friction [17], from equation 3 we see that greater Φ suggest grains with larger friction coefficient. For a given ϕ , a greater Φ can also be associated to greater heterogeneity of voids at the grain level. In the limit $\Phi \rightarrow 0$, from equation 3 we get $\phi_{rlp} = 2/3$. This value for ϕ_{rlp} correspond to smooth grains. A gamma distribution of Voronoi lenghts [20] is obtained for $K_{rlp} \approx 20$ (see figure 1). The invariant distribution found in experiments by Aste *et al* for spheres packings in mechanical equilibrium is also a gamma distribution [2].

It have been reported that at a packing fraction near the ϕ_{rlp} found by us the process of compaction is slowed. Before reaching ϕ_e , typically we have four differents regimes as we record the evolution of the packing fraction in a Monte Carlo simulation of the PLM [18]. During a first stage, ϕ “... increases rapidly until a value of around 0.65” [18], and from this point afterwards the increase in ϕ is considerably slower. Thus, ϕ_{rlp} can play a role in the onset of jamming in granular materials, as have been speculated in reference [19].

We introduce now a parameter ρ which is, basically, the quotient between Z given by equation 2 and Z_t which is the configurational integral without the restriction of having a definite value of A , *i.e.* when only the first δ in equation 2 is considered. This leads to:

$$\rho(\phi, \Phi) = \exp(s - s_t), \quad (4)$$

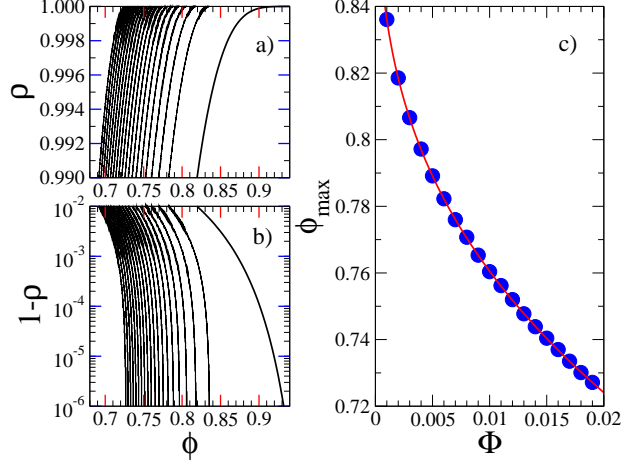


Figure 2: a) Parameter ρ (eq. 4) as a function of packing fraction ϕ for different values of the insertion probability Φ . From right to left: $\Phi = 0, 0.001, 0.002, \dots, 0.018, 0.019$. b) $1-\rho$ on a logarithmic scale as a function of ϕ for different values of Φ (same data than in a)). From the intersection with the horizontal axis we can estimate the maximum value of packing fraction ϕ_{max} for a given Φ . c) Circles: ϕ_{max} vs. Φ as obtained from b). When $\phi \rightarrow \phi_{max}$, then $\rho \rightarrow 1$. The solid line is equation 1, the steady state relation between ϕ and Φ .

with $s_t = \phi + \phi \ln \left(\frac{1-\phi}{\phi} \right)$ [9] and the entropy density s is given by equation 6 in the Appendix. In figure 2a we can see $\rho(\phi, \Phi)$. For a given value of Φ , $\rho \rightarrow 1$ as ϕ is increased up to a maximum value ϕ_{max} . This maximum value of ϕ can be estimated from a graph like the one shown in figure 2b.

In figure 2c it can be seen that $\rho \rightarrow 1$ is equivalent to say that we are approaching a steady state situation. With this in mind, in figure 3 we plot the insertion probability Φ vs. the packing fraction ϕ for a given value of the parameter ρ . We did this by solving numerically the relevant equations needed for to evaluate equation 4. It is worth to remember that a (ϕ, Φ) statistical description for the PLM makes sense only if we need to consider configurations out of steady state, since in steady state these two variables are related by equation 1. Thus, configurations with $\rho < 1$ are.

3 Discussion

In the last stages of a Monte Carlo simulation of the PLM ϕ is increasing into ϕ_e with a small variation in the insertion probability Φ . Talbot, Tarjus and Viot found in reference [15] that for $K > K_c \approx 100$, there is a minimum in Φ as a function of time that occurs at a packing fraction $\phi_m(K)$. This implies that for slow compaction if $K > K_c$ the system can increase its packing fraction while increasing or decreasing Φ , depending if ϕ is greater or smaller than ϕ_m . This should have consequences for *processes* (curves) in a (ϕ, Φ) plane like the one shown in figure 3. Thus, for $\phi > \phi_{rlp}$ in the PLM we have two zones in which we expect different behaviour. In terms of K these zones are: $K_{rlp} < K < K_c$ and $K > K_c$, with $K_{rlp} \approx 20$ and $K_c \approx 100$.

In reference [21] the authors reported a phase transition when inserting slowly a rod into a column of grains: the system's response to shear changes at a certain packing fraction ϕ_c . ϕ_c can be localized by monitoring the change in height Δh of the column, after removing the rod, as a function of ϕ [21]. It would be interesting to put the results of reference [21] in terms of a process that starts from a packing fraction ϕ_i on the $\rho = 1$ curve of figure 3 and ends on a packing fraction ϕ_f , with $\phi_i > \phi_f$ [21].

Can this two-variable description of the PLM be related to the volume-stress proposal of Edwards and others? We believe that a connection can be made by using a quantity analog to $\rho(\phi, \Phi)$ given by equation 4 as the order parameter in the stress tensor σ_{ij} proposed by Aranson and Tsimring in their

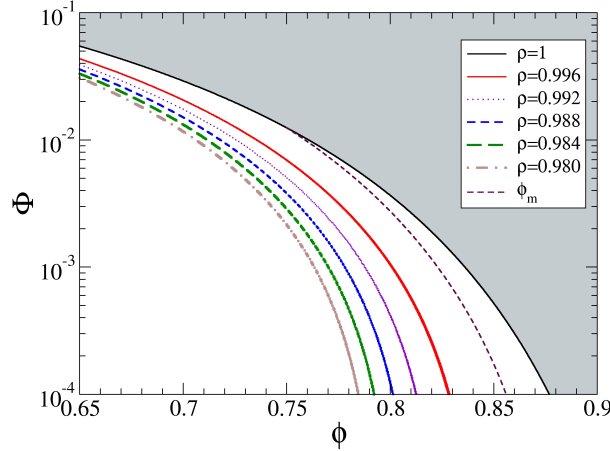


Figure 3: Insertion probability Φ vs packing fraction ϕ for different values of the parameter ρ . The particular case $\rho = 1$ is given by equation 1, the steady state relation between ϕ and Φ . The dark region are not available (ϕ, Φ) configurations and its frontier is defined by the $\rho = 1$ curve. Configurations with $\rho < 1$ age. The dotted line is a schematic representation of $\phi_m(K)$ [15].

continuum description of slow and dense granular flows [10, 11]:

$$\sigma_{ij} = \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \sigma_{ij}^0 [\rho + (1 - \rho)\delta_{ij}], \quad (5)$$

where σ_{ij}^0 is the stress under static conditions with the same geometry. Thus, ρ in eq. 4 can control how fluid and solid is the form for the stress tensor. For $\rho < 1$ we have a partially fluidized granular medium. At best, this is a first step, a suggestion, towards a real connection between Edwards' statistical mechanics and granular hydrodynamics [22].

Finally, since configurations with $\rho < 1$ in the PLM age we must say something about the relevant time scales for this model. Kolan, Nowak and Tkachenko have found that the low relaxation frequency ω_L and the high relaxation frequency ω_H for this model are given by $\omega_L = \frac{2p_+}{\delta_e} \exp(-2/\delta_e)$ and $\omega_H = p_+ \delta$, with $\delta = (1 - \phi)/\phi$ [14]. Thus, in order to speak of thermodynamic processes in figure 3, the observation time t_{obs} [23] must satisfy $1/\omega_H \ll t_{obs} \ll 1/\omega_L$. From figure 5 of reference [14], we can see that this condition on t_{obs} can be satisfied only for high packing fractions. Only for $K > K_c$ we have at least two orders of magnitude of separation between ω_L and ω_H .

4 Conclusion

We have obtained in this article the random loose packing fraction ϕ_{rlp} for the parking lot model, where ϕ_{rlp} is the lower packing fraction in which we can find a sample in mechanical equilibrium. We have done this by taking the limit of infinite compactivity in the statistical description of Tarjus and Viot, in which a macro state is characterized by its packing fraction ϕ and its insertion probability Φ . The compactivity χ is the analog of temperature in the statistical mechanics for granular materials proposed by Edwards. We have proposed an order parameter $\rho(\phi, \Phi)$ that characterizes how far from a steady situation the model is. Thus, configurations with $\rho < 1$ age. With ρ , we proposed a connection of statistical mechanics with the continuum description of slow and dense granular flows by Aranson and Tsimring. By considering the relevant time scales for this model obtained by Kolan, Nowak and Tkachenko, we have argued that for blocked configurations ($\phi > \phi_{rlp}$), only for even higher packing fractions we expect to be able to speak of thermodynamic processes for this model.

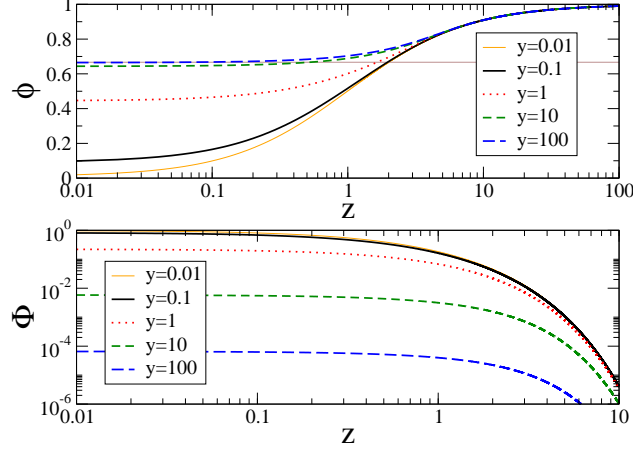


Figure 4: Equations 29 and 30 of reference [9]. For a given insertion probability Φ , we have a maximum z , which implies a maximum packing fraction ϕ_{max} . The horizontal line corresponds to $\phi = 2/3$, the maximum random loose packing fraction for the PLM (see eq. 3).

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6 Appendix

Tarjus and Viot obtained the entropy density $s(\phi, \Phi)$ ($Z = \exp(Ls)$) (eq. 28 in [9]):

$$s = (1 - \phi)z + y\Phi + \phi \ln \left(\frac{z + y[1 - \exp(-z)]}{z(z + y)} \right) \quad (6)$$

with $z = z(\phi, \Phi)$ and $y = y(\phi, \Phi)$ being solutions to the coupled equations 29 and 30 of reference [9], which can be seen in figure 4. We have that $z = (\partial S / \partial L)_{N,A}$ can be interpreted as the inverse of compactivity and $y = (\partial S / \partial A)_{N,L}$.

We can obtain the random loose packing fraction of this model by considering the limit $z \rightarrow 0$ ($\chi \rightarrow \infty$) [3, 4, 5] in equations 29 and 30 of reference [9]. We obtain:

$$\Phi = \frac{1}{(1 + y) \left[1 + y + \frac{y^2}{2(1+y)} \right]} \quad (7)$$

and

$$\frac{1}{\phi_{rlp}} = 1 + \frac{1}{y} + \frac{y}{2(1+y)} \quad (8)$$

from which we can eliminate y to obtain $\phi_{rlp}(\Phi)$, as can be seen in the inset of figure 1.

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